# Identifying Particle Interaction Features that Drive Clustering in Dense Suspensions

DMS-2201627
DMR-2410985

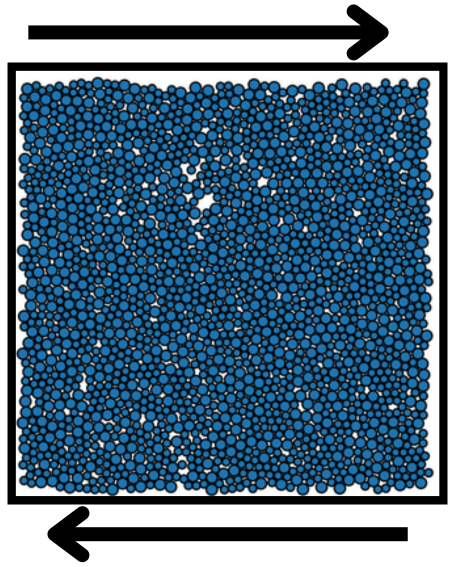
K. Gadgil, I. Malek, J. Jaquette, L. Cummings, and L. Kondic, Dept. Mathematical Sciences, NJIT
A. Brolin, R. Pandare, J. Morris, Dept. of Chemical Engineering, CCNY
M. Orsi, Polytechnic University of Turin

NJIT Grace Hopper AI Research Institute Seed Program

## Introduction

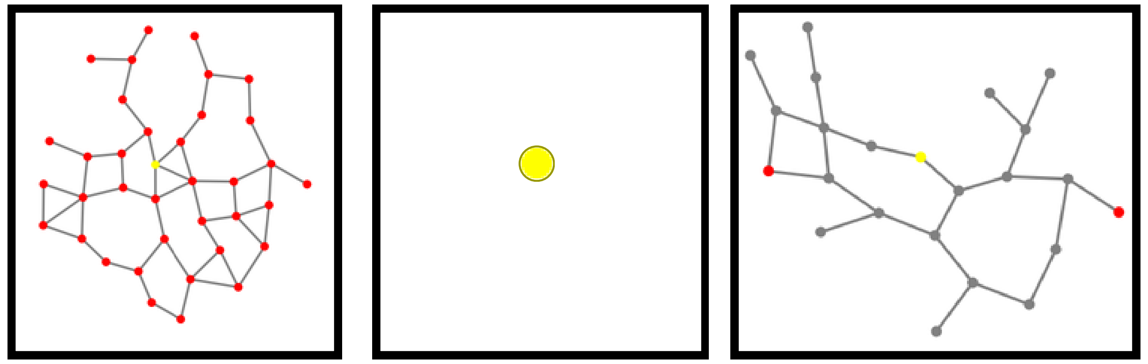
**Dense suspensions** consist of solid particles packed closely in a fluid. As the shear stress upon the system increases, the suspension undergoes shear thickening, where viscosity increases. This increase in viscosity is caused by the formation of **rigid clusters** (particles that are locked together through frictional contact).

In this project, particle interaction features are used to train a machine learning model that predicts what particles are part of rigid clusters. The data used is obtained by generating cluster labels with the pebble game for 2D simulations created using LFDEM.



## Methods

Particle contact in dense suspensions can be presented as graphs where the particles are nodes and the frictional contact between particles are edges. To view local structure information, the **swatch-cloth** method is used where a **swatch** is a small sub-network centered around a **particle** (node), extending out to four layers of contacts for neighboring particles.




These are sample swatches where a center node (yellow) is in frictional contact with particles in rigid clusters (red) and particles not in rigid clusters (grey).

## Model

A Random Forest Classification model was trained using the number of particles per layer, the average degree per layer, and the standard deviation of the degrees per layer in each swatch for each simulation to predict a particle's cluster identity. 80% of swatches were used for training while 20% for testing of the model. The model results for each shear stress dependent simulation are seen below.

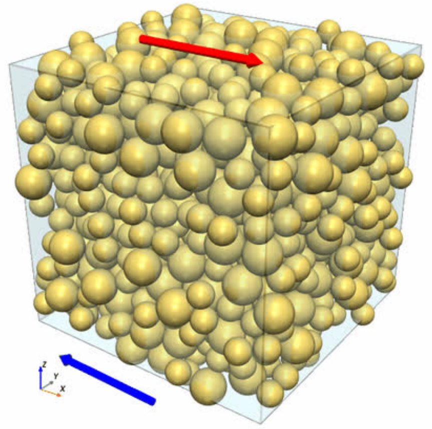
| Shear Stress ($\sigma$) | Accuracy (%) | TP | TN | FP | FN |
|---|---|---|---|---|---|
| 1 | 99.99 | 85 | 400277 | 27 | 11 |
| 2 | 99.28 | 11227 | 386290 | 1254 | 1629 |
| 5 | 91.22 | 300661 | 65930 | 25948 | 7861 |
| 10 | 99.33 | 357514 | 40209 | 1977 | 700 |

## Application

Knowing which particles are most likely to form clusters and to what capacity for a material allows for products like cement or paint to be designed such that they flow smoothly and without particles jamming, and this can also help refine protective gear that stiffens on impact and prevents injuries.

## Next Steps

We aim to extend this analysis to 3D simulations, where identifying rigid clusters is difficult because current algorithms are slow and often inaccurate. Creating a model that can reliably predict clustering in 3D would allow the modeling and study of realistic systems.



Presented by
Kinjal Gadgil